

Perfluorododecanoic acid
307-55-1 | DTXSID8031861

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 103 °C

Global applicability domain: Outside

Local applicability domain index: 2.57e-01

Confidence level: 6.11e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Perfluorododecanoic acid</div> <div>Measured: 108</div> <div>Predicted: 103</div>	<div>Image not found</div> <div>PFOA</div> <div>Measured: 55.0</div> <div>Predicted: 53.2</div>	<div>Image not found</div> <div>1-Nonanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-hexadecafluoro-</div> <div>Measured: 56.0</div> <div>Predicted: 54.2</div>
<div>Image not found</div> <div>Sulfluramid</div> <div>Measured: 96.0</div> <div>Predicted: 92.5</div>	<div>Image not found</div> <div>Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-</div> <div>Measured: 34.0</div> <div>Predicted: 32.9</div>	